

CONTENTS OF VOLUME 81

NUMBER 1—JANUARY 1994

Sub-Doppler supersonic jet spectra of the coupled $6a_0^1$ and $6b_0^1$ vibronic bands of the $S_1(^1B_{2u}) \leftarrow S_0(^1A_{1g})$ transition in monodeuterobenzene and their rovibrational analysis	1
By E. RIEDLE, A. BEIL, D. LUCKHAUS and M. QUACK	1
Effective oscillator strengths and transition energies for the hydrogen molecular ion	17
By J. F. BABB	17
High resolution CARS spectroscopy of molecular nitrogen up to 1000 bar	31
By P. ROLLAND, B. POULIGNY, E. MORIN, A. MENIL and J. P. DEJEAN	31
Square-well dimers of different bond lengths. Theory and simulation for the equation of state	43
By A. THOMAS and M. D. DONOHUE	43
Incoherent quasi-elastic neutron scattering study of highly oriented fibres of copper laurate in the columnar mesophase	57
By M. BÉE, A. M. GIROUD-GODQUIN, P. MALDIVI and J. WILLIAMS	57
Continuum resonance Raman scattering in isotopically pure $^{127}\text{I}^{35}\text{Cl}$. Determination of excited state potential functions	69
By M. GANZ and W. KIEFER	69
Correlated and gauge origin independent calculations of magnetic properties. I. Triply bonded molecules	87
By S. P. A. SAUER, I. PAIDAROVÁ and J. ODDERSHEDE	87
Molecular structure and vibrational infrared spectra of formaldehyde, selenoformaldehyde and their dihalogenoderivatives by <i>ab initio</i> post-Hartree-Fock calculation	119
By J. S. KWIATKOWSKI and J. LESZCZYŃSKI	119
An improved potential model for n-hexadecane molecular dynamics simulations under extreme conditions	133
By S. CHYNOWETH and Y. MICHOPOULOS	133
The influence of concentration and ionic strength on the cluster structure of highly charged electrolyte solutions	143
By J. L. F. ABASCAL, F. BRESME and P. TURQ	143
Frequency-dependence of second refractivity virial coefficients of small molecules between 325 nm and 633 nm	157
By U. HOHM	157
Coupled wavepackets study of the dynamics of a model ion-molecule charge exchange	169
By F. AGUILLO, V. SIDIS and J. P. GAUYACQ	169
Computer simulation study of a highly polar fluid under the influence of static electric fields	199
By P. G. KUSALIK	199
Neutron diffraction study of heavy water steam	217
By U. BUONTEMPO, P. POSTORINO, M. A. RICCI and A. K. SOPER	217
Modelling surface reconstructions with glue Hamiltonians	227
By K. D. HAMMONDS	227
The entropy of a network crystal, fluid and glass	237
By R. J. SPEEDY and P. G. DEBENEDETTI	237

CONTENTS OF VOLUME 81

NUMBER 2—10 FEBRUARY 1994

Non-equilibrium molecular dynamics calculation of heat conduction in liquid and through liquid–gas interface	251
By T. IKESHOJI and B. HAFSKJOLD	
The isotropic to nematic crystal transition for hard ellipsoids: an Onsager-like theory and computer simulations	263
By A. SAMBORSKI, G. T. EVANS, C. P. MASON and M. P. ALLEN	
Effects of a core electric dipole moment on Rydberg states	277
By J. K. G. WATSON	
Spectra of the rare gas hydrides V: the <i>np</i> Rydberg series of KrD	291
By I. DABROWSKI and D. A. SADOVSKII	
Molecular dynamics simulation of the infrared spectrum of ultrafast interconverting geometrical isomers	327
By S. WEISS, M. BUCHNER and TH. DORFMÜLLER	
Product operator theory for <i>ABX</i> spin systems and its application to H–C–C INEPT NMR experiments	337
By TOSHIHITO NAKAI and C. A. McDOWELL	
Electric resonance optothermal spectrum of the $920\text{ cm}^{-1} v_{14} + v_{15}$ torsional combination band of acetaldehyde	359
By S. BELOV, G. T. FRASER, J. ORTIGOSO, B. H. PATE and M. YU. TRETYAKOV	
Studies of $\text{U}(\text{C}_6\text{H}_5)_3\text{Cl}$: reorientational motions of cyclopentadienyl rings	369
By P. RAISON, G. H. LANDER, A. DELAPALME, J. H. WILLIAMS, R. KAHN, C. J. CARLILE and B. KANELLAKOPULOS	
A perturbative treatment of fluctuating polarizability in classical fluids	385
By J. S. HOYE and E. LOMBA	
Infrared spectroscopy of fluoride molecules in noble gas solutions. I. Octahedral molecules	395
By SH. SH. NABIEV and V. D. KLIMOV	
Structure and dynamics of molten aluminium and gallium trihalides. II. Raman spectroscopy and <i>ab initio</i> calculations	409
By A. D. ALVARENGA, M.-L. SABOUNGI, L. A. CURTISS, M. GRIMSDITCH and L. E. MCNEIL	
An improved He–CO interaction potential from a multiproperty analysis	421
By F. A. GIANTURCO, N. SANNA and S. SERNA-MOLINERA	
Time dependent wavepackets and periodic orbit assignment	447
By SEON-WOOG CHO and M. S. CHILD	
Comparison of positional disorder in the liquid and glassy states of hydrocarbons: dependence of disorder on molecular shape	467
By A. CHAKRABARTI, S. YASHIONATH and C. N. R. RAO	
Anomalous diffusion in confined monolayer films	475
By M. SCHOEN, J. H. CUSHMAN and D. J. DIESTLER	
A comparison between kinetic theory and affine transformation theory for self diffusion in a fluid of aligned hard spheroids	491
By B. KUMAR and A. J. MASTERS	

NUMBER 3—20 FEBRUARY 1994

<i>Ab initio</i> potential energy curves and binding energies of Ar_2 and Mg_2	507
By FU-MING TAO and YUH-KANG PAN	
A memory function approach to the shape of pressure broadened molecular bands	519
By G. BIRNBAUM	
Electric field effects on the carbon-13 nuclear magnetic shielding in several organic molecules	533
By M. GRAYSON and W. T. RAYNES	

CONTENTS OF VOLUME 81

Investigations of the pressure broadening of OCS and CO rotational lines in the millimetre wave range using a new type of Fourier transform spectrometer	547
By J. DOOSE, H. MÄDER, R. SCHWARZ and A. GUARNIERI	
Polarizabilities of aromatic six-membered rings: azines and 'inorganic benzenes'	557
By E. F. ARCHIBOND and A. J. THAKKAR	
Self-diffusion in the plastic phase of succinonitrile by ^2H NMR quadrupole echo train	569
By A. GOLEMME, S. ZAMIR, R. POUPKO, H. ZIMMERMANN and Z. LUZ	
Non-additive intermolecular forces from the spectroscopy of van der Waals trimers: far-infrared spectra and calculations on $\text{Ar}_2\text{-DCI}$	579
By M. J. ELROD, R. J. SAYKALLY, A. R. COOPER and J. M. HUTSON	
Near critical phase behaviour of dilute mixtures	599
By M. T. GUIDE and A. S. TEJA	
Molecular tunnelling in <i>p</i>-tert-butylcalix[4]arene(2:1)<i>p</i>-xylene	609
By M. PRAGER, R. CACIUFO, G. AMORETTI, C. J. CARLILE, G. CODDENS, F. FILLAUX, O. FRANCESCANGELI and F. UGOZZOLI	
Vibronic interaction in multielectronic mixed-valence trimeric clusters	621
By S. I. BOLDYREV, V. YA. GAMURAR, B. S. TSUKERBLAT and A. V. PALII	
Analytical treatment of the quadratic and nonrelativistic Renner-Teller effect for a triatomic molecule in a Π electronic state. III. Intermediate limit case ($\epsilon \lesssim 1 \ll m \sim E^{2/3}$) and comparison with semiclassical results	655
By A. AGUILAR, M. GONZÁLEZ and L. V. POLUYANOV	
Energies and widths of the quasibound levels of the HD^+ molecule	667
By T. ORLIKOWSKI	
Molecular dynamics simulation of semi-flexible mesogens	675
By M. R. WILSON	
Capillary condensation in non-uniform pores. Density functional approach	691
By C. CHMIEL, K. KARYKOWSKI, A. PATRYKIEW, W. RŻYSKO and S. SOKOŁOWSKI	
Dielectric spectroscopy and molecular dynamics of $\text{CH}_3\text{Cl}/\text{CCl}_4$ liquid solutions	705
By T. GROCHULSKI and A. KOCOT	
Reactive canonical Monte Carlo. A new simulation technique for reacting or associating fluids	717
By J. K. JOHNSON, A. Z. PANAGIOTOPoulos and K. E. GUBBINS	
A real function representation for the structure of the hard-sphere fluid	735
By J. CHANG and S. I. SANDLER	
A completely analytic perturbation theory for the square-well fluid of variable well width	745
By J. CHANG and S. I. SANDLER	

NUMBER 4—MARCH 1994

A generalized heat flow algorithm	767
By D. P. HANSEN and D. J. EVANS	
Computer modelling of the structure of 4-n-octyl-4'-cyanobiphenyl adsorbed on graphite	781
By D. J. CLEAVER and D. J. TILDESLEY	
Theory and computer simulation of hard-sphere site models of ring molecules	801
By R. P. SEAR and G. JACKSON	
Calculation of orientation-dependent double-tensor moments for Coulomb-type intermolecular interactions	813
By C. HÄTTIG and B. A. HED	
Theoretical study of the activation of methane by photoexcited zinc atoms	825
By S. CASTILLO, A. RAMÍREZ-SOLÍS, D. DÍAZ, E. POULAIN and O. NOVARO	
A test of the modified Enskog theory for self-diffusion	837
By J. M. KINCAID, R.-F. TUO and M. LOPEZ DE HARO	
Second virial coefficients of chain molecules: A Monte Carlo study	851
By V. I. HARISMIADIS and I. SZLEIFER	

CONTENTS OF VOLUME 81

Phase transitions in thin films of symmetric binary polymer mixtures		
By S. K. KUMAR, HAI TANG and I. SZLEIFER		867
Adiabatic potential of the system of two equivalent vibronic centres with common atoms. I.		
One-centre-coordinate approach		
By L. F. CHIBOTARU		873
Adiabatic potential of the system of two equivalent vibronic centres with common atoms. II.		
Equilibrium nuclear configurations of the bioctahedral systems		
By L. F. CHIBOTARU		891
The Coulson-Fischer $+r_{12}$ wavefunction for H_2		
By N. J. CLARKE, D. L. COOPER, J. GERRATT and M. RAIMONDI		921
The electronic structure of the dipolar atomic state in a centrosymmetric environment		
By N. C. PYPER, C. G. PIKE and P. P. EDWARDS		937
A new NMR method for measuring the rotational correlation time of molecules in the liquid state		
By H. DESVAUX and M. GOLDMAN		955
Rotational quantization of methyl groups in a rotating frame		
By S. CLOUGH, A. J. HORSEWILL, M. R. JOHNSON, J. H. SUTCLIFFE and I. B. I. TOMSAH		975
On the damped multipole expansion of the induction energy in H_2^+		
By G. FIGARI, C. COSTA, A. SICILIANO and V. MAGNASCO		991
Measurement of the first excited bending state of Ar-CO using a new concentration modulation technique in the jet		
By M. HAVENITH, G. HILPERT, M. PETRI and W. URBAN		1003
Research Note		
How reliable is the HMSA integral equation for the pair structure of supercooled and amorphous mixtures?		
By F. OULD-KADDOUR and G. PASTORE		1011

NUMBER 5—10 APRIL 1994

Molecular order and dynamics of the nemogen MBBA. Modelling of deuterium NMR observables		
By R. Y. DONG, L. FRIESEN and G. M. RICHARDS		1017
Calculation of second virial coefficients of alkanes with the MM2 and MM3 force fields		
By J. NAGY, V. H. SMITH, JR. and D. F. WEAVER		1039
Depolarization-density tuning in supracritical solutions of methane-carbon dioxide		
By E. J. ROSE and F. G. BAGLIN		1049
Interfacial tension in confined molecularly-thin films		
By J. E. CURRY, J. H. CUSHMAN, M. SCHOEN and D. J. DIESTLER		1059
Quantum Monte Carlo simulation of molecular vibrations. Application to formaldehyde		
By M. LEWERENZ and R. O. WATTS		1075
Adhesive-hard-sphere approximation for the structure of square-well fluids: application to colloidal dispersions		
By K. SHUKLA and R. RAJAGOPALAN		1093
Cross-polarization dynamic-angle spinning nuclear magnetic resonance of quadrupolar nuclei		
By J. H. BALTSISBERGER, S. L. GANN, P. J. GRANDINETTI and A. PINES		1109
Proton two-dimensional exchange nuclear magnetic resonance study of a p-xylene-d zeolite inclusion compound		
By A. KUBO, A. K. DUBEY and C. A. McDOWELL		1125
Molecular dynamics simulation of the liquid mixtures CCl_4/CS_2. II. Concentration dependence of the translational and rotational motion		
By U. MITTAG, J. SAMIOS and TH. DORFMÜLLER		1143
Computer simulations do not support Cl-Cl pairing in aqueous NaCl solution		
By G. HUMMER, D. M. SOUMPASIS and M. NEUMANN		1155
The phase transitions of sulphur hexafluoride by molecular dynamics simulation		
By A. BOUTIN, J. M. SIMON and A. H. FUCHS		1165

CONTENTS OF VOLUME 81

The microwave spectrum and molecular structure of ethylisocyanate	
By N. HEINEKING, J.-U. GRABOW and W. STAHL	1177
A systematic study of the structure of liquid iso-propanol by time-of-flight neutron diffraction	
By P. ZETTERSTRÖM, U. DAHLBORG and W. S. HOWELLS	1187
The microwave spectrum and equilibrium conformation of phthalan	
By L. A. LEAL, J. L. ALONSO, D. G. LISTER and J. C. LÓPEZ	1205
Vibrational frequency shifts in NeHF and ArHF complexes	
By S. A. C. McDOWELL, M. G. TREFRY and A. D. BUCKINGHAM	1225
The pathways of the combined Cope rearrangement–molecular reorientation process in solid bullvalene: a deuterium 2D exchange NMR study on a single crystal	
By A. MÜLLER, U. HABERLEN, H. ZIMMERMANN, R. POUPKO and Z. LUZ	1239

Research Notes

Neutron diffraction investigation of the structure of the C₃D₃ film physisorbed upon MgO(100)	
By A. COULOMB, Y. LARHER, M. TRABELEI and I. MIREBEAU	1259
Correlation energy of diatomic molecules versus number of electrons	
By A. GRASSI, G. M. LOMBARDO, N. H. MARCH and P. PUCCI	1265

NUMBER 6—20 APRIL 1994

Atom–atom potential energy calculations for the absorption of cations in muscovite	
By P. PAVLIDES and C. R. A. CATLOW	1269
Molecular dynamics study of an isomerizing triatomic in solution	
By S. WEISS	1281
Non-equilibrium molecular dynamics calculation of thermal conductivity of flexible molecules: butane	
By P. J. DAIVIS and D. J. EVANS	1289
Study of the Feynman–Hibbs effective potential against the path-integral formalism for Monte Carlo simulations of quantum many-body Lennard-Jones systems	
By L. M. SESÉ	1297
Structure and thermodynamics of heteronuclear two-centre Lennard-Jones fluids from Monte Carlo simulation and a reference hypernetted chain equation	
By M. LOMBARDERO, C. MARTÍN and E. LOMBA	1313
Transport and relaxation properties of N₂	
By E. L. HECK and A. S. DICKINSON	1325
High-frequency interaction-induced rototranslational wings of isotropic nitrogen spectra	
By T. BANCEWICZ, V. TEBOL and Y. LE DUFF	1353
Comment on ‘Theoretical calculations of the nuclear magnetic shielding tensors for the ethylenic carbon atoms in cyclopropenes’	
By CH. VAN WÜLLEN, U. FLEISCHER and W. KUTZELNIGG	1373
Analysis of $\tilde{\Delta}^2A_1-\tilde{C}^2T_2$ emission bands of CF₃⁺ under high resolution	
By J. F. M. AARTS and J. H. CALLOMON	1383
The molecular structure of the (NCCN)₂ and (PCCP)₂ van der Waals dimers	
By W. B. DE ALMEIDA, S. M. RESENDE and H. F. DOS SANTOS	1397
Helical motions of aliphatic chains in molecular crystals. The incoherent quasi-elastic neutron scattering law	
By F. GUILLAUME	1411
Non-additive three-body interaction energies for H₃ (quartet spin state)	
By Z. C. ZHANG, A. R. ALLNATT, J. D. TALMAN and W. J. MEATH	1425
Diode laser spectroscopy of the 7i–6h and 7h–6g transitions in H₂	
By F. J. BASTERRECHEA, P. B. DAVIES, D. M. SMITH and R. J. STICKLAND	1435
Theoretical study of the Renner–Teller $\tilde{\Delta}^2A_1-\tilde{X}^2B_1$ system of NH₂	
By W. GABRIEL, G. CHAMBAUD, P. ROSMUS, S. CARTER and N. C. HANDY	1445

CONTENTS OF VOLUME 81

Tunnelling in the A $^1\Pi$ state and the dissociation energy of BH By M. PERSICO	1463
Numerical solution of the RHNC theory for water-like fluids near a macroparticle and a planar wall By M. KINOSHITA and M. HARADA	1473
A nonplanar cyclic minimum-energy structure of singlet C₉ By Z. SLANINA, S.-L. LEE, J.-P. FRANÇOIS, J. KURTZ, L. ADAMOWICZ and M. SMIGEL ..	1489
 Research Note	
Scaling properties of inhomogeneity kinetic energy in some diatomic molecules, in relation to dissociation energies By G. J. LAMING, A. NAGY, N. C. HANDY and N. H. MARCH	1497
Index of authors (with the titles of papers)	1501

